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APPROXIMATE
SERIES SOLUTIONS
OF THE THREE-SPECIES
ATMOSPHERIC DEIONIZATION
DIFFERENTIAL EQUATIONS

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APPROXIMATE SERIES SOLUTIONS OF THE
THREE-SPECIES ATMOSPHERIC DEIONIZATION
DIFFERENTIAL EQUATIONS

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RM 65TMP-7
1 February 1965

This research has been sponsored by the Defense
Atomic Support Agency under NWER Subtask
07.028, Contract DA 49-146-XZ-281

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ABSTRACT

In the course of investigating the effects of a nuclear explosion on electromagnetic wave propagation, it is often convenient to consider the ionized constituents of the atmosphere to be represented by a single species of positive ions, a single negative ion species, and electrons. The number densities of these charged particles at a specific time after detonation are then obtained from the solution of a system of three differential equations which describe the time rate of change of each particle density. An exact analytic solution has not been found for these equations, and hence either approximate analytic forms or numerical integration methods are employed. The latter offers high accuracy but is often too time-consuming for general application. In this report a new set of approximate analytic solutions are derived which provide accuracies approaching that of numerical integration for many cases, but which retain the advantage of rapid computation.

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INTRODUCTION

An essential part of an investigation of the effects of nuclear explosions on electromagnetic wave propagation is the determination of atmospheric ionization produced by energy released by the detonation. Once the level of initial ionization, produced by the almost instantaneous energy pulse, and the continuing rate of ion production, resulting from beta and gamma radiation accompanying the radioactive decay of the fission debris, have been determined from the burst parameters and atmospheric transmission properties, the problem becomes one of obtaining a solution to the system of differential equations which describe the time rate of change of the number density of each atmospheric constituent. Well over a hundred different reactions involving a dozen or more different atmospheric species may be included in the general problem. Keneshea [Ref. 1] has investigated this problem and has developed a digital computer program which employs numerical integration methods to treat a system of thirteen variable species involving 131 reactions.

When many different altitudes must be considered under varying conditions of initial ionization and ionization source strength, it is often not feasible to consider the general problem, and some means of approximating the physical situation with a simpler mathematical model is needed. Furthermore, many of the coefficients which specify the rates at which the various reactions proceed are poorly known at best, thus reducing the need for a rigorous treatment of the problem in many investigations. One approach which is widely used consists of employing three variable species to represent the ones actually present: a single positive ion species, a single negative ion species, and electrons. The neutral population is considered to be constant at any given altitude. These three species are allowed to participate in four reactions: recombination of electrons with positive ions, mutual neutralization of positive and negative ions, attachment of electrons to neutrals, and detachment of electrons from negative ions. As in the more general approach, charge balance is maintained (the positive ion density equals the sum of the electron and negative ion densities).

The problem is therefore reduced to a system of three simultaneous, first-order, nonlinear differential equations. Even this reduced system is still difficult to solve analytically, and resort must be made to either numerical methods or approximate solutions.* When a large number of calculations must be made, approximate analytic solutions are often preferred for their relative simplicity and ease of computation. The disadvantage of such solutions has been the limited accuracy of the results obtained from them under certain combinations of parameters. It is an unfortunate fact that most of the approximate solutions exhibit their poorest accuracy in cases involving altitudes between roughly 50 km and 80 km, which is precisely where the need for accuracy is the greatest since most of the propagation disturbances due to a nuclear detonation are maximum at these altitudes.

The mathematical difficulty which is encountered in attempting to solve the deionization equations analytically is due primarily to unequal rates for the dissociative recombination and mutual neutralization reactions — if these reactions are assumed to proceed at equal rates, the deionization equations may be solved exactly for certain source functions. However, most of the current estimates of the rate coefficients give values for these two reactions which differ by factors ranging from about 4 to 10. Hence it is necessary to have available solutions which provide for this difference.

The need for such solutions became acute in preparing the revised edition of the Electromagnetic Blackout Handbook [Ref. 2]. The large number of calculations which were necessary to produce graphical material for the Handbook made the use of numerical methods of solution prohibitively expensive. On the other hand, the approximate analytic solutions in use at that time were known to have poor accuracy in certain regimes. It was apparent that a need existed for new approximations giving higher accuracy but retaining the essential characteristic of rapid computation.

The derivation of the approximate analytic solutions which were used in preparation of material for the Handbook is presented in this report. In addition to the assumption that the reaction rate coefficients are constant at any given altitude, there are two

* See the note at the end of this report for reference to a recent Lincoln Laboratory report which describes a computer solution employing numerical integration methods.

approximations inherent in the derivation: both the ionization source strength and an effective positive ion recombination coefficient, which will be defined, are assumed independent of time. The effect of these approximations will be illustrated as will methods of reducing the inaccuracy they produce. It will be seen that although the solutions can be used for an occasional hand calculation, they are best suited for rapid machine computation. A Fortran-coded computer program employing the solutions is available [Ref. 3].

DERIVATION OF THE SOLUTIONS

The differential equations which describe the three-species system may be written as

$$\frac{dN_e}{dt} = q - \alpha_d N_e N_+ - A N_e + D N_- \quad (1)$$

$$\frac{dN_-}{dt} = -\alpha_i N_- N_+ + A N_e - D N_- \quad (2)$$

$$\frac{dN_+}{dt} = q - \alpha_i N_- N_+ - \alpha_d N_e N_+ \quad (3)$$

where

N_e = number density of electrons

N_- = number density of negative ions

N_+ = number density of positive ions

q = rate of ion production (source strength)

α_d = dissociative recombination reaction rate coefficient

α_i = mutual neutralization reaction rate coefficient

A = attachment rate coefficient

D = detachment rate coefficient

These equations satisfy the charge-balance relation

$$N_+ = N_e + N_- \quad (4)$$

If we define an effective positive ion recombination coefficient as

$$\alpha = \frac{N_- \alpha_i + N_e \alpha_d}{N_+} \quad (5)$$

then the positive ion differential equation becomes

$$\frac{dN_+}{dt} = q - \alpha N_+^2 \quad (6)$$

We now introduce the approximations that q and α are independent of time, in which case the solution of (6) is found to be

$$N_+(t) = \sqrt{\frac{q}{\alpha}} \frac{1 + Ce^{-2\sqrt{q\alpha}t}}{1 - Ce^{-2\sqrt{q\alpha}t}} \quad (7)$$

where

$$C = \frac{N_+(0) - \sqrt{\frac{q}{\alpha}}}{N_+(0) + \sqrt{\frac{q}{\alpha}}} \quad (8)$$

Using (4) to eliminate N_- from (1) and substituting (7) for N_+ , the electron density differential equation becomes

$$\begin{aligned} \frac{dN_e}{dt} = & q + D\sqrt{\frac{q}{\alpha}} \frac{1 + Ce^{-2\sqrt{q\alpha}t}}{1 - Ce^{-2\sqrt{q\alpha}t}} \\ & - \left(A + D + \alpha_d \sqrt{\frac{q}{\alpha}} \frac{1 + Ce^{-2\sqrt{q\alpha}t}}{1 - Ce^{-2\sqrt{q\alpha}t}} \right) N_e \quad (9) \end{aligned}$$

This is a linear equation with variable coefficients, and the solution may be obtained in integral form through classical methods:

$$N_e(t) = \frac{e^{-\left(A+D\sqrt{\frac{\alpha_d}{\alpha}}\sqrt{q\alpha}\right)t}}{\left(1-Ce^{-2\sqrt{q\alpha}t}\right)^{\alpha_d/\alpha}} \left\{ \int e^{\left(A+D\sqrt{\frac{\alpha_d}{\alpha}}\sqrt{q\alpha}\right)t} \left[q\left(1-Ce^{-2\sqrt{q\alpha}t}\right)^{\alpha_d/\alpha} + D\sqrt{\frac{q}{\alpha}} \left(1-Ce^{-2\sqrt{q\alpha}t}\right)^{\alpha_d/\alpha-1} \left(1+Ce^{-2\sqrt{q\alpha}t}\right) \right] dt + K \right\} \quad (10)$$

where K is a constant to be determined from the initial conditions.

The integral in (10) may readily be obtained in closed form if $\alpha = \alpha_d$. The result is sometimes termed the "equal-alpha" solution.* The equal-alpha solution applies therefore to cases in which the dissociative recombination and mutual neutralization reaction rate coefficients are equal, and to cases in which the negative ion population is negligible with respect to the electron (and positive ion) population. This latter situation arises when the rate of electron attachment is small relative to the rate at which negative ions are lost through detachment and mutual neutralization. Since this occurs in the daytime ionosphere above, say, 80 km or at roughly the same altitudes in the nighttime ionosphere for fairly large ion production rates, it is seen that the equal-alpha solution can be essentially an exact solution of the three-species system (except for the constant-q approximation) for certain cases of interest even when α_i and α_d are not assumed to be equal.

When α does not coincide with α_d , the integral in (10) is not so easily obtained. Applying the binomial expansion to the troublesome factors and grouping terms, the integral in (10) may be put in the following form:

* The well-known result for $\alpha = \alpha_d$ is

$$N_e(t) = \left(1 - Ce^{-2\sqrt{q\alpha}t}\right)^{-1} \left\{ (1-C) N_e(0) e^{-(A+D\sqrt{q\alpha})t} + \frac{q+D\sqrt{\frac{q}{\alpha}}}{A+D\sqrt{q\alpha}} \left[1 - e^{-(A+D\sqrt{q\alpha})t} \right] - C \frac{q-D\sqrt{\frac{q}{\alpha}}}{A+D\sqrt{q\alpha}} \left[e^{-2\sqrt{q\alpha}t} - e^{-(A+D\sqrt{q\alpha})t} \right] \right\} \quad (11)$$

$$\begin{aligned}
& \int e^{(A+D+k\sqrt{q\alpha})t} \left\{ q + D\sqrt{\frac{q}{\alpha}} - C \left[kq + (k-2)D\sqrt{\frac{q}{\alpha}} \right] e^{-2\sqrt{q\alpha}t} \right. \\
& + \frac{C^2}{2!} (k-1) \left[kq + (k-4)D\sqrt{\frac{q}{\alpha}} \right] e^{-4\sqrt{q\alpha}t} \\
& - \frac{C^3}{3!} (k-1)(k-2) \left[kq + (k-6)D\sqrt{\frac{q}{\alpha}} \right] e^{-6\sqrt{q\alpha}t} \\
& \left. + \frac{C^4}{4!} (k-1)(k-2)(k-3) \left[kq + (k-8)D\sqrt{\frac{q}{\alpha}} \right] e^{-8\sqrt{q\alpha}t} - \dots \right\} dt
\end{aligned}$$

where

$$k = \frac{\alpha_d}{\alpha} \quad (12)$$

This expansion is convergent for $|Ce^{-2\sqrt{q\alpha}t}| \leq 1$, which is always true, and hence may be integrated term by term. After evaluating the constant K, the resulting solution for N_e is

$$\begin{aligned}
N_e(t) = & \left(1 - Ce^{-2\sqrt{q\alpha}t}\right)^{-k} \left\{ (1-C)^k N_e(0) e^{-(A+D+k\sqrt{q\alpha})t} \right. \\
& + \frac{q+D\sqrt{\frac{q}{\alpha}}}{A+D+k\sqrt{q\alpha}} \left[1 - e^{-(A+D+k\sqrt{q\alpha})t} \right] \\
& - C \frac{kq+(k-2)D\sqrt{\frac{q}{\alpha}}}{A+D+(k-2)\sqrt{q\alpha}} \left[e^{-2\sqrt{q\alpha}t} - e^{-(A+D+k\sqrt{q\alpha})t} \right] \\
& + \frac{C^2}{2!} (k-1) \frac{kq+(k-4)D\sqrt{\frac{q}{\alpha}}}{A+D+(k-4)\sqrt{q\alpha}} \left[e^{-4\sqrt{q\alpha}t} - e^{-(A+D+k\sqrt{q\alpha})t} \right] \\
& - \frac{C^3}{3!} (k-1)(k-2) \frac{kq+(k-6)D\sqrt{\frac{q}{\alpha}}}{A+D+(k-6)\sqrt{q\alpha}} \left[e^{-6\sqrt{q\alpha}t} - e^{-(A+D+k\sqrt{q\alpha})t} \right] \\
& + \dots \\
& + \frac{(-C)^n}{n!} (k-1)(k-2)\dots(k-n+1) \frac{kq+(k-2n)D\sqrt{\frac{q}{\alpha}}}{A+D+(k-2n)\sqrt{q\alpha}} \left[e^{-2n\sqrt{q\alpha}t} - e^{-(A+D+k\sqrt{q\alpha})t} \right] \\
& \left. + \dots \right\} \quad (13)
\end{aligned}$$

It may be seen that for $k = 1$, equation (13) reduces to the equal-alpha solution, equation (11), as would be expected.

The same procedure used to obtain this result may also be applied to the negative ion density differential equation (2). Usually, however, an adequate solution for the negative ion density may be obtained through the charge-balance equation (4). This can result in some numerical inaccuracy when the positive ion and electron concentrations are nearly equal, but in such cases there is usually little need for great accuracy in the negative ion density solution.

Equations (7) and (13) are general solutions to the three-species system, subject only to the two approximations inherent in their development. Before turning to an examination of the effect of these approximations, it is worthwhile to consider some potential computational difficulties which may arise in applying these results and how the difficulties can be avoided.

In computing electron density from (13), enough terms are included in the series until the contribution of succeeding terms becomes negligible. Usually this requires only a few terms, although the exact number needed in a particular case depends on the values of the parameters. For cases in which the term $D\sqrt{\frac{q}{\alpha}}$ is large compared to q , which may occur for low source strengths in the daytime, it is possible to observe a false null in the series which should not be interpreted as indicating that sufficient terms have been included. This occurs when k is nearly equal to $2n$, where $n = 1, 2, 3, \dots$, and results from the small magnitude of the term having $(k - 2n)D\sqrt{\frac{q}{\alpha}}$ in the numerator. Even though this term may be negligible, the next term which involves $(k - 2n - 2)D\sqrt{\frac{q}{\alpha}}$ will probably be significant. Thus the term following the first term which is negligible should be examined before the decision is made to terminate the series.

A more serious difficulty arises if use is made of (7) and (13) in cases where the source strength q is very small. Both (7) and (13) become indeterminate for vanishing q , and hence are useless for computational purposes in such cases. To handle these cases it is necessary to develop additional forms for the solutions. The solution for the positive ion density when q is of negligible

importance may be obtained either by taking the limit of (7) as $q \rightarrow 0$, or by solving (6) after eliminating q . The solution is found to be

$$N_+(t) = \frac{N_+(0)}{1 + \alpha N_+(0)t} \quad (14)$$

A new solution for the electron density may now be obtained after substituting (14) for N_+ in the differential equation. Equation (1) becomes

$$\frac{dN_e}{dt} = q + \frac{DN_+(0)}{1 + \alpha N_+(0)t} - \left(A + D + \frac{\alpha_d N_+(0)}{1 + \alpha N_+(0)t} \right) N_e \quad (15)$$

Note that q has been left in the electron density differential equation. This is done since cases arise in practice wherein the source strength is an important term in the electron density equation even though it has a negligible effect on the positive ion density. This situation is most likely to occur after a large initial level of ionization in the nighttime at fairly low altitudes where attachment rates are large. The inclusion of q in (15) does not lead to any computational difficulty for the case where $q = 0$. As before, the solution of (15) may be obtained in integral form through classical techniques:

$$N_e(t) = \frac{e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^{\frac{\alpha_d}{\alpha}}} \left\{ \int_0^t e^{(A+D)t} \left(q [1 + \alpha N_+(0)t]^{\frac{\alpha_d}{\alpha}} + DN_+(0) [1 + \alpha N_+(0)t]^{\frac{\alpha_d}{\alpha} - 1} \right) dt + K \right\} \quad (16)$$

As was the case previously, the integration is readily performed in closed form if $\alpha = \alpha_d$, yielding the equal-alpha electron density solution for small q .* When α and α_d are unequal, equation (16)

* The solution of (16) for $\alpha = \alpha_d$ is

$$N_e(t) = \frac{N_e(0) e^{-(A+D)t}}{1 + \alpha N_+(0)t} + \frac{N_+(0) [D(A+D) - q\alpha]}{(A+D)^2} \left[\frac{1 - e^{-(A+D)t}}{1 + \alpha N_+(0)t} \right] + \frac{q}{A+D} \left[1 - \frac{e^{-(A+D)t}}{1 + \alpha N_+(0)t} \right] \quad (17)$$

may be put into a form suitable for computation through repeated integration by parts. Two such expansions are possible, and each has application. For cases such that

$$1 + \alpha N_+(0)t \leq 2 \frac{\alpha N_+(0)}{A+D},$$

the following convergent expansion is useful:

$$\begin{aligned}
 N_e(t) = & \frac{N_e(0) e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^k} + \frac{D}{k\alpha} \left(1 - \frac{e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^k} \right) \\
 & + \frac{k\alpha - D(A+D)}{k(k+1)\alpha^2 N_+(0)} \left\{ \left(1 + \alpha N_+(0)t - \frac{e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^k} \right) \right. \\
 & - \frac{1}{k+2} \left[\frac{A+D}{\alpha N_+(0)} \right] \left([1 + \alpha N_+(0)t]^2 - \frac{e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^k} \right) \\
 & + \frac{1}{(k+2)(k+3)} \left[\frac{A+D}{\alpha N_+(0)} \right]^2 \left([1 + \alpha N_+(0)t]^3 - \frac{e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^k} \right) \\
 & - \dots \\
 & + \frac{(-1)^n}{(k+2)(k+3)\dots(k+n+1)} \left[\frac{A+D}{\alpha N_+(0)} \right]^n \left([1 + \alpha N_+(0)t]^{n+1} - \frac{e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^k} \right) \\
 & + \dots \left. \right\} \tag{18}
 \end{aligned}$$

For cases such that

$$1 + \alpha N_+(0)t \geq 2 \frac{\alpha N_+(0)}{A+D},$$

the foregoing expansion converges rather slowly and hence is not very suitable for computation. In such cases the following semiconvergent expansion may be used to advantage:

$$\begin{aligned}
 N_e(t) \approx & \frac{N_+(0) e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^k} + \frac{q}{A+D} \left(1 - \frac{e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^k} \right) \\
 & + N_+(0) \frac{D(A+D) - kq\alpha}{(A+D)^2} \left\{ \left(\frac{1}{1 + \alpha N_+(0)t} - \frac{e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^k} \right) \right. \\
 & - (k-1) \frac{\alpha N_+(0)}{A+D} \left(\frac{1}{[1 + \alpha N_+(0)t]^2} - \frac{e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^k} \right) \\
 & + (k-1)(k-2) \left[\frac{\alpha N_+(0)}{A+D} \right]^2 \left(\frac{1}{[1 + \alpha N_+(0)t]^3} - \frac{e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^k} \right) \\
 & + \dots \\
 & \left. + (-1)^n (k-1)(k-2) \dots (k-n) \left[\frac{\alpha N_+(0)}{A+D} \right]^n \left(\frac{1}{[1 + \alpha N_+(0)t]^{n+1}} - \frac{e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^k} \right) \right\}
 \end{aligned}
 \tag{19}$$

This series should be terminated when either or both of the factors (k-n) or

$$\left(\frac{1}{[1 + \alpha N_+(0)t]^{n+1}} - \frac{e^{-(A+D)t}}{[1 + \alpha N_+(0)t]^k} \right)$$

change sign. It may be seen that for $k = 1$ equation (19) reduces to the equal-alpha solution valid for small q , equation (17).

The decision to use equations (14) and (18) or (19) in place of equations (7) and (13) may be made by first obtaining from (14) a lower limit of N_+ , i. e., that value of positive ion density which would result if there were no continuing source of ionization. If the ion production rate term in the positive ion differential equation (6) is insignificant compared to the term αN_+^2 using the lower limit of N_+ , then the value of N_+ obtained from (14) is the proper value and either (18) or (19) should be employed to find the electron density. Stated mathematically, equations (14), (18), and (19) are valid when

$$q \ll \alpha \left[\frac{N_+(0)}{1 + \alpha N_+(0)t} \right]^2$$

otherwise equations (7) and (13) should be used.

One other computational difficulty can occur if (13) is employed for cases involving essentially zero initial conditions, low values of q , and relatively small values of time. In such cases the initial terms in the series in (13) may be several orders of magnitude larger than the final answer, convergence is quite slow, and numerical inaccuracy may result. For this type of problem suitable approximations may be made to arrive at a closed-form expression for the electron density solution. Thus for the conditions

$$N_+(0) \ll \sqrt{\frac{q}{\alpha}}$$

$$\sqrt{q\alpha} t \ll 1,$$

we may make the following approximations

$$e^{\sqrt{q\alpha} t} - Ce^{-\sqrt{q\alpha} t} \approx 2 \quad (20)$$

$$e^{\sqrt{q\alpha} t} + Ce^{-\sqrt{q\alpha} t} \approx 2 \left[\frac{N_+(0) + qt}{\sqrt{\frac{q}{\alpha}}} \right]$$

Introducing these into the positive ion density solution (7) there results

$$N_+(t) \approx N_+(0) + qt \quad (21)$$

The integral form of the electron density solution, equation (10), reduces upon substitution of the above approximations to

$$N_e(t) \approx e^{-(A+D)t} \left\{ \int_0^t e^{(A+D)t} (q + D[N_+(0) + qt]) dt + K \right\} \quad (22)$$

Performing the integration and evaluating the constant in terms of the initial condition we obtain

$$N_e(t) \approx N_e(0) e^{-(A+D)t} + \left[\frac{q + DN_+(0)}{A+D} - \frac{Dq}{(A+D)^2} \right] \left[1 - e^{-(A+D)t} \right] + \frac{Dqt}{A+D} \quad (23)$$

Sufficient relations have now been developed to handle all situations commonly encountered in practice. It still remains, however, to provide some procedure for determining the value of α to be used in the equations. The definition of α , equation (5), is not directly usable for this purpose since it is expressed in terms of the solutions of the equations, although the initial value of α can be found from (5) using the known initial conditions:

$$\alpha(0) = \frac{\alpha_i N_i(0) + \alpha_d N_e(0)}{N_+(0)} \quad (24)$$

As $t \rightarrow \infty$, α approaches a steady-state* value which may be found by introducing the steady-state ion density solutions into (5). For this purpose it is convenient to rewrite the definition of α in terms of the ratio of negative ion density to electron density:

* In practice, the term "quasi-equilibrium" is often used instead of "steady-state" since generally the source strength q is not independent of time as has been assumed here. However, it often happens that q varies slowly enough with time so that after the initial transients die out the ion densities approach a condition where they are essentially in equilibrium with q at any given instant.

$$\alpha = \frac{\lambda \alpha_i + \alpha_d}{\lambda + 1} \quad (25)$$

where

$$\lambda = \frac{N}{N_e} \quad (26)$$

Under steady-state conditions we have from (2) and (7)

$$\lambda(\infty) = \frac{A}{D + \alpha_i \sqrt{\frac{q}{\alpha(\infty)}}} \quad (27)$$

Substituting (27) into (25) there results

$$a(\infty) = \frac{A\alpha_i + D\alpha_d + \alpha_i \alpha_d \sqrt{\frac{q}{\alpha(\infty)}}}{A + D + \alpha_i \sqrt{\frac{q}{\alpha(\infty)}}} \quad (28)$$

Equation (28) yields a cubic in α which may be solved directly, or an iterative procedure may be used. A good starting point for the iteration is provided by replacing α in the right-hand member by $(A\alpha_i + D\alpha_d) / (A+D)$. This is the limiting form of $\alpha(\infty)$ for the case of vanishing q . The values obtained through iteration converge rapidly to the solution of (28), and often the very first value furnishes an acceptable approximation to the solution.

Once the initial and final values of α have been obtained from (24) and (28) respectively, a reasonably good approximation for α at intermediate times has been found to be

$$\alpha(t) \approx \alpha(0) e^{-(A+D)t} + \alpha(\infty) [1 - e^{-(A+D)t}] \quad (29)$$

ACCURACY OF THE SOLUTIONS

The accuracy of the solutions developed in the preceding section is dependent upon the validity of the "constant-q" and "constant- α " approximations in any given situation. For those cases in which q and α exhibit little variation over the time interval of interest, the solutions are found to be quite accurate. For example, if α_d and α_i are essentially equal, or if the negative ion density is initially small relative to the electron density and remains so due to low rates of attachment, the constant- α approximation is valid and the accuracy of the solutions is dependent upon the validity of the constant-q approximation alone. The latter situation includes many of the cases encountered in the analysis of nuclear burst-produced ionization at altitudes above about 80 km.

Another type of problem for which the constant- α approximation is valid is one in which sufficient time has elapsed to attain a condition of quasi-equilibrium with a slowly varying (or constant) source. In this case α stabilizes at the value given by equation (28) and is essentially constant. The quasi-equilibrium term in equation (13),

$$N_e(\infty) = \frac{q + D\sqrt{\frac{q}{\alpha}}}{A + D + \alpha_d\sqrt{\frac{q}{\alpha}}}, \quad (30)$$

then yields a result which is an exact solution for the quasi-equilibrium case providing α is computed exactly from equation (28). Since a good solution to (28) is readily obtained using a very few iterations, quite acceptable accuracy (on the order of a few percent or better) is realized for the quasi-equilibrium case with less computation needed than by most other methods offering comparable accuracy.

A determination of the accuracy of the solutions for problems involving altitudes below about 80 km and times prior to the establishment of quasi-equilibrium is somewhat complicated by the fact that

a number of parameters are involved, each of which may range over a wide spectrum of values. The accuracy in any given situation is a function of the values of the parameters. To evaluate the approximate solutions, a number of cases have been computed and the results compared with solutions obtained through numerical integration of the deionization equations.* In general, the maximum error attributable to the constant- α approximation occurs during the attachment phase for cases in which the initial ion concentrations are large, the source strength is relatively small, attachment is a significant electron loss process, and the dissociative recombination and mutual neutralization reaction rate coefficients are appreciably different. The attachment phase may be defined as that period of time when terms involving $e^{-(A+D)t}$ are important. During this period the true value of α experiences a pronounced variation with time. At later times α is a slowly-varying quantity at worst, and hence the constant- α approximation becomes quite good.

Consider, for example, a problem defined by the following parameters:

$$N_e(0) = N_+(0) = 1 \times 10^{10} \text{ cm}^{-3}$$

$$q = 1 \times 10^4 \text{ cm}^{-3} \text{ sec}^{-1}$$

$$h = 50, 60, 70, 80 \text{ km (day and night)}$$

The reaction rate coefficients for these altitudes are taken from Reference 4 using the 1962 U.S. Standard Atmosphere for atmospheric density and temperature values. The coefficient values are listed in Table 1.

* The numerical integration was performed using a computer program written by C. Luehr, TEMPO. This program uses the SHARE library routine R W INT as its basic component. This is a Fortran version of R W -DE2F which integrates a system of N simultaneous, first order, ordinary differential equations with the option of using either 4th order Runge-Kutta method, or 4th order predictor-corrector method (Adams-Moulton) with either fixed or variable step size. Double precision is used internally to control round-off errors. The predictor-corrector method with variable step size was used to obtain the results presented in this report.

Table 1. Reaction rate coefficients used in calculations.

h (km)	α_d ($\text{cm}^3 \text{sec}^{-1}$)	α_i ($\text{cm}^3 \text{sec}^{-1}$)	A (sec^{-1})	D (day) (sec^{-1})	D (night) (sec^{-1})
50	2.586×10^{-7}	6.477×10^{-8}	5.842×10^1	0.4415	1.473×10^{-3}
60	2.738×10^{-7}	6.384×10^{-8}	4.954×10^0	0.4408	7.984×10^{-4}
70	3.188×10^{-7}	6.795×10^{-8}	3.577×10^{-1}	0.4497	1.801×10^{-3}
80	3.875×10^{-7}	7.454×10^{-8}	1.687×10^{-2}	0.4957	2.050×10^{-3}

The electron density time history for this problem, obtained through numerical integration, is presented graphically in Figures 1 and 2 for daytime and nighttime values of detachment, respectively. Numerical values of electron density at times of 0.01, 0.03, 0.1, 0.3, 1.0, 3.0, 10, 30, and 100 seconds are listed in Tables 2 and 3. The first column for each altitude contains the values given by numerical integration. These are considered exact for the purpose of evaluating the approximate analytic solutions. The second column for each altitude contains values calculated from the approximate solutions derived in the preceding section.

The comparison in Tables 2 and 3 shows that the approximate solutions exhibit relatively little error at any time at the 80-km altitude, a conclusion previously deduced from the fact that α remains essentially constant at a value near α_d at such altitudes since relatively little build-up of the negative ion density occurs. What error that does occur at 80 km is largest for the nighttime case, which is not surprising since larger negative ion densities are formed for the lower nighttime detachment.

At the 50, 60, and 70 km altitudes, the error in the approximate series solutions is seen to be a pronounced function of time, becoming quite large at certain times and then falling rapidly to

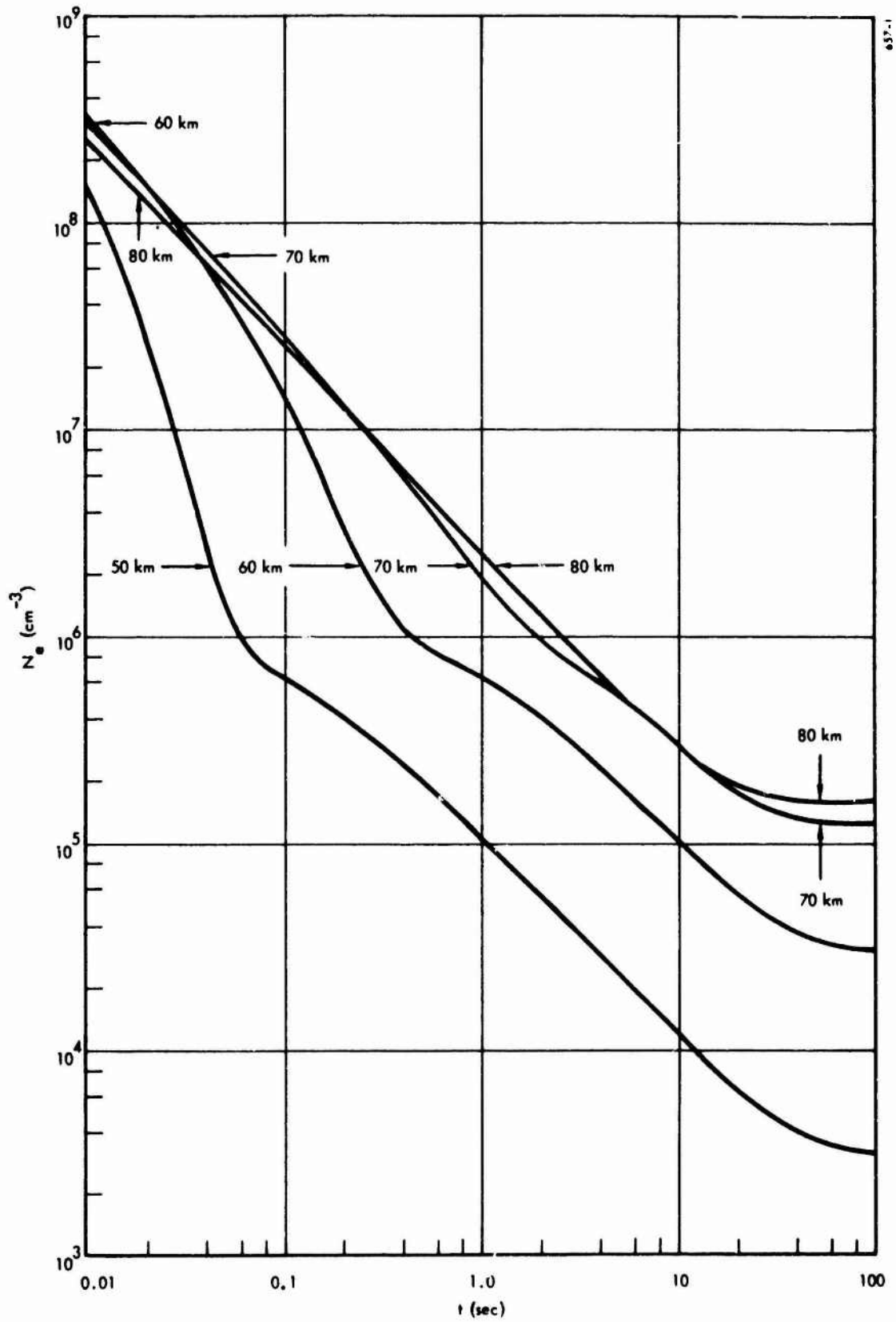


Figure 1. Numerical integration solution for $N_e(0) = N_+(0) = 1 \times 10^{10} \text{ cm}^{-3}$, $q = 1 \times 10^4 \text{ cm}^{-3} \text{ sec}^{-1}$ (daytime)

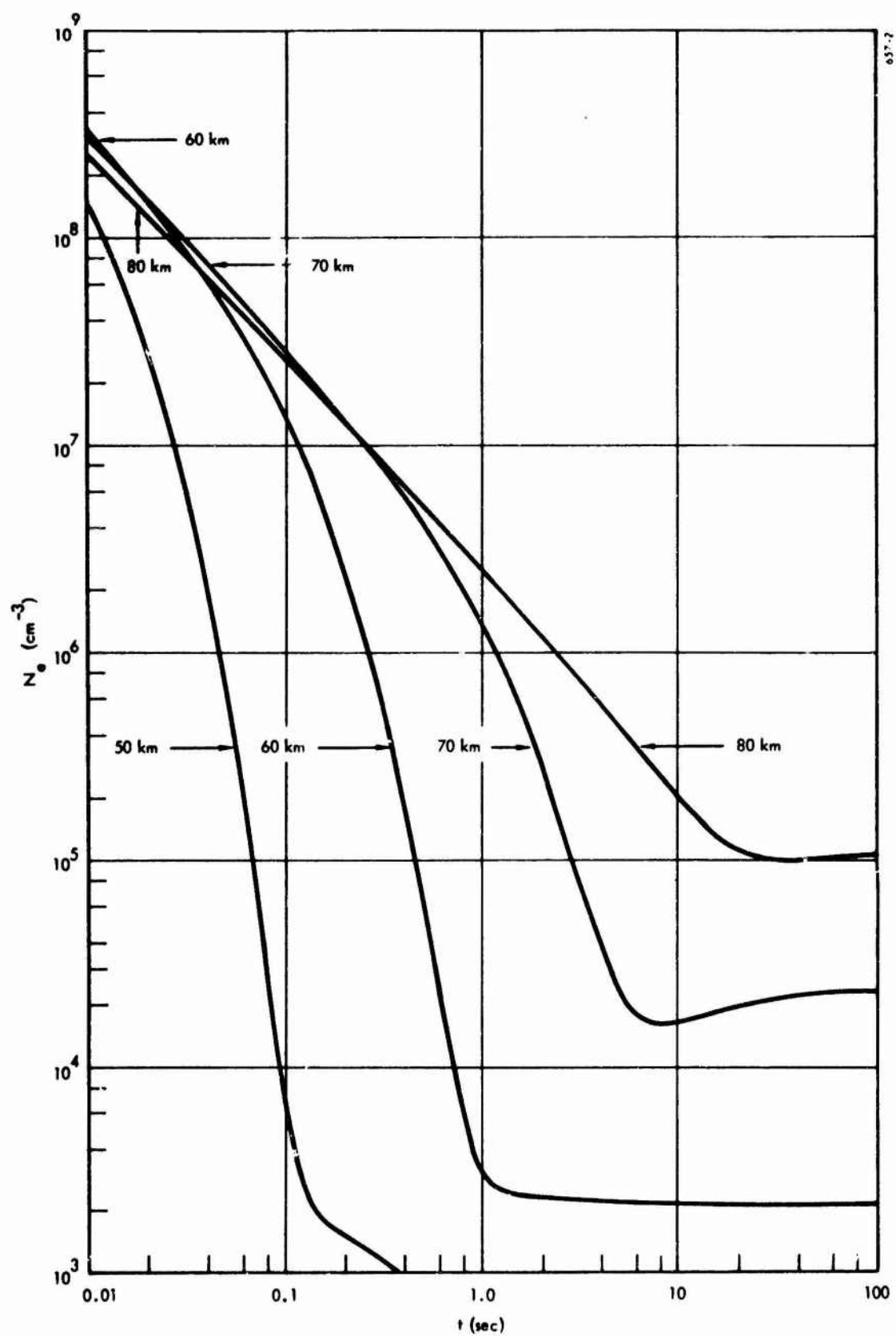


Figure 2. Numerical integration solution for $N_e(0) = N_+(0) = 1 \times 10^{10}$
 $q = 1 \times 10^4 \text{ cm}^{-3}$ (nighttime)

Table 2. Comparison of results for $N_e(0) = N_+(0) = 10^{10} \text{ cm}^{-3}$, $q = 10^4 \text{ cm}^{-3} \text{ sec}^{-1}$.
(Daytime)

t (sec)	50 km				60 km				70 km				80 km			
	Num. Int.	*	†	Equal Alpha	Num. Int.	*	†	Equal Alpha	Num. Int.	*	†	Equal Alpha	Num. Int.	*	†	Equal Alpha
0.01	1.53+8	7.34+7	1.23+8	7.33+8	3.27+8	3.07+8	3.20+8	1.05+9	3.02+8	3.01+8	3.02+8	4.58+8	2.52+8	2.51+8	2.52+8	2.58+8
0.03	8.00+6	1.32+6	5.90+6	8.50+7	9.25+7	7.04+7	8.95+7	3.41+8	1.01+8	9.95+7	1.01+8	1.56+8	8.55+7	8.51+7	8.52+7	8.76+7
0.1	6.40+5	7.17+5	6.45+5	1.53+6	1.43+7	4.69+6	1.38+7	7.53+7	2.87+7	2.67+7	2.91+7	4.63+7	2.55+7	2.55+7	2.56+7	2.64+7
0.3	3.01+5	3.21+5	3.04+5	3.76+5	1.60+6	1.05+6	1.54+6	1.08+7	8.50+6	6.42+6	8.54+6	1.45+7	8.60+6	8.39+6	8.51+6	8.79+6
1	1.06+5	1.08+5	1.06+5	1.13+5	6.35+5	6.65+5	6.06+5	1.06+6	1.94+6	1.29+6	1.99+6	3.64+6	2.52+6	2.44+6	2.52+6	2.62+6
3	3.70+4	3.72+4	3.70+4	3.79+4	2.95+5	2.90+5	2.78+5	3.38+5	7.10+5	8.52+5	7.13+5	9.65+5	8.40+5	8.30+5	8.50+5	8.71+5
10	1.16+4	1.17+4	1.16+4	1.17+4	1.01+5	9.98+4	9.84+4	1.05+5	2.92+5	2.69+5	2.65+5	2.91+5	2.90+5	2.86+5	2.86+5	2.88+5
30	4.65+3	4.66+3	4.66+3	4.67+3	4.30+4	4.20+4	4.19+4	4.31+4	1.42+5	1.39+5	1.39+5	1.44+5	1.66+5	1.66+5	1.66+5	1.66+5
100	3.11+3	3.11+3	3.11+3	3.12+3	3.01+4	3.01+4	3.01+4	3.06+4	1.23+5	1.23+5	1.23+5	1.27+5	1.58+5	1.58+5	1.58+5	1.58+5
Max. Error		83.5% 0.03 sec	26.2% 0.03 sec	962% 0.03 sec		67.2% 0.1 sec	5.8% 3 sec	575% 0.3 sec		33.5% 1 sec	9.2% 10 sec	87.6% 1 sec		3.2% 1 sec	1.4% 10 sec	4.0% 1 sec

* Approximate series solution, each time calculated separately.

† Approximate series solution, sequential calculations at times listed, starting with 0.003 sec.

NOTE: Signed numbers denote powers of 10.

Table 3. Comparison of results for $N_e(0) = N_+(0) = 10^{10} \text{ cm}^{-3}$, $q = 10^4 \text{ cm}^{-3} \text{ sec}^{-1}$.

(Nighttime)

Electron Density

t (sec)	50 km					60 km					70 km					80 km				
	Num. Int.	*	†	Equal Alpha	Num. Int.	Num. Int.	*	†	Equal Alpha	Num. Int.	Num. Int.	*	†	Equal Alpha	Num. Int.	*	†	Equal Alpha	Num. Int.	†
0.01	1.53+8	7.21+7	1.23+8	7.46+8	3.27+8	3.06+8	3.20+8	1.29+9	1.29+9	3.02+8	3.02+8	3.01+8	3.02+8	1.26+9	2.52+8	2.52+8	2.52+8	1.26+9	2.52+8	2.52+8
0.03	7.30+6	2.22+5	4.85+6	8.48+7	9.20+7	6.96+7	8.91+7	4.28+8	4.28+8	1.01+8	1.01+8	9.95+7	1.01+8	4.55+8	8.55+7	8.52+7	8.52+7	4.55+8	8.55+7	8.52+7
0.1	7.20+3	2.53+3	4.98+3	4.45+5	1.37+7	3.38+6	1.29+7	9.39+7	9.39+7	2.87+7	2.87+7	2.66+7	2.90+7	1.37+8	2.55+7	2.56+7	2.57+7	1.37+8	2.55+7	2.56+7
0.3	1.16+3	1.23+3	1.18+3	1.45+3	6.20+5	4.15+3	5.86+5	1.18+7	1.18+7	8.20+6	8.20+6	5.87+6	8.32+6	4.31+7	9.50+6	8.46+6	8.52+6	4.31+7	9.50+6	8.46+6
1	5.20+2	5.29+2	5.22+2	5.57+2	2.97+3	2.45+3	2.96+3	1.14+5	1.14+5	1.36+6	1.36+6	3.16+5	1.45+5	1.01+7	2.46+6	2.43+6	2.51+6	1.01+7	2.46+6	2.43+6
3	2.95+2	2.95+2	2.94+2	3.00+2	2.22+3	2.23+3	2.21+3	2.73+3	2.73+3	9.10+4	9.10+4	1.22+4	1.20+5	1.66+6	7.60+5	7.12+5	7.98+5	1.66+6	7.60+5	7.12+5
10	2.10+2	2.10+2	2.09+2	2.11+2	2.10+3	2.09+3	2.09+3	2.23+3	2.23+3	1.62+4	1.62+4	1.60+4	1.73+4	6.66+4	2.00+5	1.62+5	2.25+5	6.66+4	2.00+5	1.62+5
30	1.86+2	1.86+2	1.86+2	1.87+2	2.05+3	2.05+3	2.05+3	2.10+3	2.10+3	2.07+4	2.07+4	2.10+4	2.12+4	2.76+4	9.75+4	1.03+5	1.15+5	2.76+4	9.75+4	1.03+5
100	1.81+2	1.81+2	1.81+2	1.81+2	2.04+3	2.04+3	2.04+3	2.07+3	2.07+3	2.26+4	2.26+4	2.26+4	2.26+4	2.77+4	1.03+5	1.13+5	1.09+5	2.77+4	1.03+5	1.13+5
Max. Error		97.0% 0.03 sec	33.6% 0.03 sec	6080% 0.1 sec		99.3% 0.3 sec	5.8% 0.1 sec	3740% 1 sec				86.6% 3 sec	31.9% 3 sec	1720% 3 sec		19.0% 10 sec	18.0% 30 sec	1720% 3 sec		19.0% 10 sec

* Approximate series solution, each time calculated separately.

† Approximate series solution, sequential calculations at times listed, starting with 0.003 sec.

NOTE: Signed numbers denote powers of 10.

negligible values. The time of maximum error is a function of altitude, and by referring to Figures 1 and 2 the maximum error at each altitude is observed to occur during the period when the electron density is decreasing most rapidly with time. This is the "attachment phase" mentioned previously, and the error is a result of a significant variation in the value of α during this period. Note that the error becomes quite small after the attachment phase has ended, and by 100 seconds when quasi-equilibrium has essentially become established for this problem, the approximate solutions are seen to be very nearly exact at all altitudes.

Since the approximation which is responsible for the error consists of the assumption that α is a constant from the initial time to the time of calculation, we might expect that if the time interval over which the actual value of α exhibits appreciable variation were divided into several smaller time intervals, and the results at the end of each interval were used as initial conditions for the next, the error could be reduced. Such is indeed the case, and the amount by which the error is reduced is often substantial. To illustrate this, sequential calculations were performed at the times shown in Tables 2 and 3, beginning with one earlier time of 0.003 second. The values of N_e and N_+ obtained at each time were used as $N_e(0)$ and $N_+(0)$ for the next calculation. The results obtained by this procedure are presented in the third column for each altitude in Tables 2 and 3. In every case the maximum error is lower than for the separate calculations, often significantly lower. Perhaps the most striking comparison occurs for the 60-km nighttime calculation at 0.3 second. The separate calculation for this time is over 2 orders of magnitude low (the largest discrepancy found for this method of calculation), whereas the value obtained by calculating sequentially is only 5.5 percent low.

The foregoing problem was chosen for illustration since the combination of parameters it involves is representative of something approaching the worst case which is likely to be encountered in practice, as far as the accuracy of the approximate solutions is concerned. The large maximum errors found in this example are a result of the combination of the following two conditions:

- 1) unequal α_i and α_d together with significant build-up of the negative ion concentration due to relatively large attachment rates, causing a pronounced variation of α with time,

- 2) large initial electron and positive ion concentrations together with a relatively low source strength, causing the recombination terms to be important in both the positive ion and electron density differential equations and hence making the precise value and time history of α important.

Tests can be inferred from these conditions which may be used to predict which cases are likely to be subject to significant errors. Thus, cases which satisfy all three of the following tests are suspect:

$$\begin{aligned} \alpha &\neq \alpha(0) \\ \alpha N_p(0)t &\gg 1, \\ (A+D)t &\leq \frac{\alpha_d}{\alpha} \end{aligned} \tag{31}$$

These tests may be applied before the approximate series solutions are employed at a specific time in a particular problem, and if all three are satisfied a good solution may be obtained by computing at one or two earlier times, using the results at each earlier time as initial conditions for the next time interval. This method is employed in the computer program described in Reference 3.

While the maximum inaccuracy in these approximate series solutions may appear to be large, and indeed it is for single-time calculations under certain conditions, it should be noted that over much of the time interval of interest in nuclear weapons effects studies the error is quite small in this problem, and the solutions will be found to be better for different problems involving lower initial conditions. Another point to be considered is that even in this problem the series approximations are generally much better than other, simpler analytic approximations which are commonly used. One such approximation is the equal-alpha solution, equations (11) and (17). The equal-alpha solution is often used with a value of alpha taken as $(A\alpha_1 + D\alpha_d)/(A+D)$. To show the comparison between this solution and the series approximations, values of electron density for the foregoing problem have been obtained from the equal-alpha solution using the above expression for alpha. These values are presented in the fourth column for each altitude in Tables 2 and 3. Although the percent error comparison is somewhat misleading since the equal-alpha solutions err on the high side while the series solutions exhibit their primary inaccuracy on the low side, examination of Table 2 and 3 reveals that, in general,

the error in the equal-alpha solutions is greater than that of the series solutions and persists over a longer time period. Furthermore, there does not appear to be a simple method of reducing the error in the equal-alpha solutions, whereas the error in the series solutions may be readily reduced by the sequential calculation procedure.

It is interesting to consider a second problem for which one of the tests which may be used to predict regions of inaccuracy in the series solutions is never satisfied:

$$N_e(0) = N_+(0) = 0$$

$$q = 1 \times 10^4 \text{ cm}^{-3} \text{ sec}^{-1}$$

$$h = 50, 60, 70, 80 \text{ km (day and night)}$$

This is the same as the first problem considered except for the initial conditions. The comparison of the numerical integration results with those obtained from separate calculations using the series solutions is shown in Tables 4 and 5 for daytime and nighttime detachment, respectively. It is seen that for this type of problem the series solutions are good to within a few percent at all times and all altitudes. No need exists to perform sequential calculations to obtain good accuracy in this case; the solution at any time is essentially unchanged if calculations are performed sequentially.

The discussion thus far has considered the effect of the constant- α approximation for several combinations of parameters. A similar discussion applies if the source strength q exhibits significant variation over the problem time interval. In such cases it is possible to reduce the inaccuracy resulting from the constant- q approximation by performing a series of calculations during the period of significant q -variation, using the results obtained at each time as initial conditions for the next calculation. For many problems encountered in nuclear weapons effects studies, however, the source strength does not vary rapidly enough with time to warrant special treatment. Exceptions to this wherein sequential calculations may be necessary because of q -variation include cases where beta-ray ionization is present at some times but not at others, and cases involving a relatively rapid variation in the gamma-ray source due to changing atmospheric mass between the source and the point of interest. Another situation wherein it may be necessary to perform sequential

Table 4. Comparison of results for $N_e(0) = N_+(0) = 0$, $q = 10^4 \text{ cm}^{-3} \text{ sec}^{-1}$.
(Daytime)

t (sec)	50 km			60 km			70 km			80 km		
	Num. Int.	*		Num. Int.	*		Num. Int.	*		Num. Int.	*	
0.01	7.55+1	7.58+1		9.75+1	9.75+1		9.98+1	9.98+1		1.00+2	1.00+2	
0.03	1.42+2	1.42+2		2.79+2	2.79+2		2.98+2	2.98+2		3.00+2	3.00+2	
0.1	1.76+2	1.75+2		7.80+2	7.89+2		9.70+2	9.80+2		9.99+2	9.96+2	
0.3	1.91+2	1.91+2		1.60+3	1.60+3		2.83+3	2.83+3		2.99+3	2.97+3	
1.0	2.44+2	2.43+2		2.50+3	2.47+3		8.60+3	8.75+3		9.92+3	1.00+4	
3.0	3.91+2	3.93+2		4.15+3	4.14+3		2.15+4	2.17+4		2.90+4	2.94+4	
10	9.03+2	9.02+2		9.65+3	9.62+3		5.65+4	5.68+4		8.65+4	8.67+4	
30	2.05+3	2.06+3		2.13+4	2.14+4		1.08+5	1.10+5		1.50+5	1.50+5	
100	3.04+3	3.04+3		2.97+4	2.97+4		1.23+5	1.23+5		1.58+5	1.58+5	
Max. Error		0.5%			1.2%			1.8%			1.4%	

* Approximate series solution, each time calculated separately.

NOTE: Signed numbers denote powers of 10.

Table 5. Comparison of results for $N_e(0) = N(0) = 0$, $q = 10^4 \text{ cm}^{-3} \text{ sec}^{-1}$.
(Nighttime)

Electron Density

t (sec)	50 km		60 km		70 km		80 km	
	Num. Int.	*	Num. Int.	*	Num. Int.	*	Num. Int.	*
0.01	7.50+1	7.57+1	9.60+1	9.75+1	9.98+1	9.98+1	1.00+2	1.00+2
0.03	1.41+2	1.41+2	2.77+2	2.79+2	2.98+2	2.98+2	3.00+2	3.00+2
0.1	1.71+2	1.70+2	7.80+2	7.86+2	9.70+2	9.80+2	9.99+2	9.96+2
0.3	1.71+2	1.71+2	1.57+3	1.55+3	2.83+3	2.82+2	2.99+3	2.97+3
1.0	1.71+2	1.71+2	2.00+3	1.96+3	8.40+3	8.16+3	9.80+3	9.90+3
3.0	1.72+2	1.72+2	2.02+3	2.02+3	1.82+4	1.83+4	2.90+4	2.89+4
10	1.74+2	1.74+2	2.02+3	2.02+3	2.58+4	2.58+4	8.10+4	8.19+4
30	1.77+2	1.77+2	2.03+3	2.03+3	2.42+4	2.41+4	1.24+5	1.24+5
100	1.81+2	1.81+2	2.04+3	2.04+3	2.27+4	2.27+4	1.09+5	1.13+5
Max. Error		0.9%		2.0%		2.9%		3.7%

* Approximate series solution, each time calculated separately.

NOTE: Signed numbers denote powers of 10.

calculations occurs if fireball radiance causes the total detachment rate coefficient D to vary appreciably with time.

The approximate solutions presented here are intended primarily for rapid machine computation. While they can be used for hand calculation, their principal advantage lies in the fact that they can be used to obtain solutions of higher accuracy than that obtainable from simpler approximate solutions, and with a much lower expenditure in computational time than that required by numerical integration methods. When applied to machine computation, it is a relatively simple task to program the machine to sense regions wherein the accuracy may be inadequate and automatically perform a few calculations at earlier times to improve the accuracy. In this manner, the solutions appear to be capable of producing acceptably accurate results for all types of problems.

NOTE ADDED IN PROOF

During the proofing of this report for publication, the author was privileged to receive a copy of a Lincoln Laboratory report describing work of a similar nature carried out jointly by Mt. Auburn Associates and M.I.T. Lincoln Laboratory. The report "A Model and a Computer Program for Atmospheric Deionization at Early Times Following Nuclear Explosions" by Frederick L. Ek [Project Report PA-77 (BMRS), 24 December 1964] is concerned with basically the same problem as that considered here — methods of obtaining acceptably accurate solutions to the system of differential equations which describe the complex atmospheric deionization processes. As is the case here, the treatment is concerned primarily with the three-species lumped-parameter system.

Whereas the approach here is one of obtaining approximate analytic solutions so as to avoid the necessity of employing numerical integration techniques, the method described by Ek is to use numerical integration to solve the time-varying portion of the problem, switching to steady-state analytic solutions at times where these are sufficiently close to the numerical solution. The numerical integration method is the same as that used here to check the accuracy of the series solutions (the same SHARE numerical integration subroutine is employed). One feature of the computer program described by Ek is that both the source strength and the detachment rate coefficient are allowed to be functions of time.

It still appears that the series solutions developed here can be used to fill the void hitherto existing between simple "equal-alpha"-type approximations on the one hand, and precise numerical integration on the other. The fact that regions of inaccuracy may be detected a priori and the solutions easily improved is believed to be a very real advantage. This combined with the relatively insignificant increase in computer time required by the series solutions over simpler and less accurate approximate solutions appears to make

the former particularly well suited for application in computer programs such as TEMPO's WEPH [Ref. 3] and perhaps Lincoln Laboratory's BOOM.

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